Curriculum Vitae

Christopher Knight, Assistant Computational Scientist
Argonne National Laboratory

Work Address

Leadership Computing Facility
Argonne National Laboratory
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Appointments

Position	*Institution (Contact)*	*Dates*
Assistant Computational Scientist	Argonne LCF (Nichols Romero)	9/2013 - present
Joint Appointment	U. Chicago Computation Institute	5/2012 - present

Postdoctoral Appointments

Institution	*Supervisor*	*Dates*
Argonne National Laboratory	Gregory A. Voth	4/2010 - 9/2013
University of Chicago	Gregory A. Voth	4/2010 - 10/2010
University of Utah	Gregory A. Voth	4/2009 - 3/2010

Education

Institution (Preceptor)	*Degree*	*Date*	*Field*
The Ohio State University (Sherwin J. Singer)	Ph.D.	2009	Chemistry
Eastern Michigan University	B.S. w/ Honors	2003	Chemistry

Honors

ANL Computational Postdoctoral Fellowship	2011-2012
Ohio State University Presidential Fellowship	2008-2009
Undergraduate Honors Senior Thesis/Project and Symposium	2003
ACS Organic Chemistry Achievement Award	2002
Honors Undergraduate Fellowship	2002
Maurice Decoster Chemistry Scholarship	2002

Professional Societies and Activities

Member of the American Chemical Society
Member of the Electrochemical Society
Referee for *seven* scientific journals: Journal of Physical Chemistry, Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, Molecular Physics, Journal of Chemical Physics, AIP Advances, and Chemical Physics Letters.

Teaching & Work Experience

ALCF Catalyst: At the ALCF (9/13-present), I work closely with researchers to help them accomplish their scientific goals on both new and mature projects using leadership computational resources. To address the unique challenges of efficiently using leadership-scale resources at ACLF, I assist researchers with porting, profiling, and debugging their codes, discuss strategies and provide general guidance on code parallelization, I/O, load-balancing, workflow design, and data management. Important components of this work are training users on key high-performance computing topics and collaborating to advance their scientific mission.

Guest Lectures at Harvard University: In Nov. 2015, I organized and presented lectures and a hands-on lesson in large-scale scientific computing as part of a course titled "APCOMP 290R - Extreme Computing: Project-based High Performance Distributed and Parallel Systems" at Harvard University with Sadasivan Shankar, Pavlos Protopapas, and Efthimios Kaxiras. I led six sessions, which included running jobs on Mira at ALCF, to illuminate how supercomputers can be used to address real-world problems, such as designing better batteries using kinetic Monte Carlo.

Mentored undergraduate and high school students
Center for Multiscale Theory and Simulation, University of Chicago (6/12-7/12)

Teaching Assistant
Department of Chemistry, The Ohio State University (9/03-9/04, 9/05-9/06)

Research Interests

- High-performance scientific computing
- Statistical mechanics
- Computer simulations via first principle methods
- Classical and quantum dynamics and multiscale processes in condensed phases
- Accurate and efficient simulation of chemical reactions in condensed phases
- Chemistry at interfaces: aqueous systems, batteries and supercapacitors (electrolyte/electrode), fuel cells (proton and hydroxide conductance), biofuels (carboxysome), and smart materials (self-healing, piezoelectric, magnetostrictive), nanoporous materials
- Interactions of matter with soft and hard X-ray pulses

Publications: 647 citations; h-index 14; i10-index 17 (April 2017)

1. Hasan Metin Aktulga, Chris Knight, Paul Coffman, Tzu-Ray Shan, and Wei Jiang, "Optimizing the Performance of Reactive Molecular Dynamics Simulations for Multi-core Architectures", *Int. J. High Perform. Comput. Appl.* (*submitted*)

2. Phay Ho and Chris Knight, "Large-scale Atomistic Calculations of Cluster in Intense X-ray Pulses", *J. Phys. B: At. Mol. Opt. Phys.* (*accepted*)

3. C. Huy Pham, Sandeep K. Reddy, Karl Chen, Chris Knight, and Francesco Paesani, "Many-Body Interactions in Ice", *J. Chem. Theory Comput.*, **13**:1778-1784 (2017)

4. Andrew D. White, Chris Knight, Glen M. Hocky, and Gregory A. Voth, "Improved Ab Initio Molecular Dynamics by Minimally Biasing with Experimental Data", *J. Chem. Phys.*, **146**:041102 (2017)

5. Phay J. Ho, Chris Knight, Miklos Tegze, Gyula Faigel, C. Bostedt, and Linda Young, "Atomistic three-dimensional coherent x-ray imaging of nonbiological Systems", *Phys. Rev. A*, **94**:063823 (2016).

6. Sandeep K. Reddy, Shelby C. Straight, Pushp Bajaj, C. Huy Pham, Marc Riera, Daniel R. Moberg, Miguel A. Morales, Chris Knight, Andreas W. Götz, and Francesco Paesani, "On the accuracy of the MB-pol many-body potential for water. I. Interaction energies, vibrational frequencies, and classical thermodynamic and dynamical properties from clusters to liquid water and ice", *J. Chem. Phys.*, **145**:194504 (2016) (2016 JCP Editor's Choice)

7. Evgenii O. Fetisov, I-F. Will Kuo, Chris Knight, Joost VandeVondele, Troy Van Voorhis, and J. Ilja Siepmann, "First Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors", *ACS Cent. Sci.*, **2**(6):409-415 (2016)

8. Chen Chen, Ying-Lung Steve Tse, Gerrick E. Lindberg, Chris Knight, and Gregory A. Voth, "Hydroxide Solvation and Transport in Anion Exchange Membranes", *J. Am. Chem. Soc.*, **138**(3):991-1000 (2016)

9. Revati Kumar, Chris Knight, Collin D. Wick, and Bin Chen, "Bringing Reactivity to the Aggregation-Volume-Bias Monte Carlo Based Simulation Framework: Water Nucleation Induced by a Reactive Proton", *J. Phys. Chem. B*, **119**(29):9068-9075 (2015)

10. Peng Bai, Mi Yeong Jeon, Limin Ren, Chris Knight, Michael W. Deem, Michael Tsapatsis, and J. Ilja Siepmann, "Discovery of optimal zeolites for challenging separations and chemical transformations using predictive materials modeling", *Nature Commun.*, **6**:5912 (2015)

11. Ying-Lung Steve Tse, Chris Knight, and Gregory A. Voth, "An Analysis of Hydrated Proton Diffusion in Ab Initio Molecular Dynamics", *J. Chem. Phys.*, **142**:014104 (2015)

12. Alistar Ottochian, Guilhem Dezanneau, Clement Gilles, Paolo Raiteri, Chris Knight, and Julian D. Gale, "Influence of isotropic and biaxial strain on proton conduction in Y-doped $BaZrO_3$: a reactive molecular dynamics study", *J. Mat. Chem. A*, **2**(9):3127-3133 (2014).

13. Revati Kumar, Chris Knight, and Gregory A. Voth, "Exploring the Behavior of the Hydrated Excess Proton at Hydrophobic Interfaces", *Farad. Discuss.*, **167**:263-278 (2013)

14. Takefumi Yamashita, Yuxing Peng, Chris Knight, and Gregory A. Voth, "Computationally Efficient Multiconfigurational Reactive Molecular Dynamics", *J. Chem. Theory Comput.*, **8**(12):4863-4875 (2012) (Berny Schlegel Festschrift)

15. Chris Knight, Gerrick E. Lindberg, and Gregory A. Voth, "Multiscale Reactive Molecular Dynamics", *J. Chem. Phys.*, **137**(22):22A525 (2012) (Nonadiabatic Dynamics special issue)

16. Chris Knight and Gregory A. Voth, "Coarse-graining Away Electronic Structure: A Rigorous Route to Accurate Condensed Phase Interaction Potentials", *Mol. Phys.*, **110**(9-10):935-944 (2012) (Bill Miller special issue).

17. Chris Knight and Gregory A. Voth, "The Curious Case of the Hydrated Proton", *Acc. Chem. Res.*, **45**(1):101-109 (2012) (Water in Chemistry special issue).

18. Sherwin J. Singer and Chris Knight, "Hydrogen bond topology and proton ordering in ice and water clusters", *Adv. Chem. Phys.*, **147**:1 (2012).

19. Hui Zhang, Ali A. Hassanali, Yun Kyung Shin, Chris Knight, and Sherwin J. Singer, "The water-amorphous silica interface: Analysis of the Stern layer and surface conduction", *J. Chem. Phys.*, **134**(2):024705 (2011).

20. Ali Hassanali, Hui Zhang, Chris Knight, Yun Kyung Shin, and Sherwin J. Singer, "The dissociated amorphous silica surface: Model development and evaluation", *J. Chem. Theory Comput.*, **6** (11):3456 (2010).

21. Chris Knight, C. Mark Maupin, Sergei Izvekov, and Gregory A. Voth, "Defining condensed phase reactive force fields from *ab initio* molecular dynamics simulations: The case of the hydrated excess proton", *J. Chem. Theory Comput.*, **6**(10):3223 (2010).

22. Chris Knight and Sherwin J. Singer, "Site disorder in ice VII arising from hydrogen bond fluctuations", *J. Phys. Chem. A*, **113**(45):12433 (2009) (Russell Pitzer Festschrift).

23. Chris Knight and Sherwin J. Singer, "Hydrogen bond ordering in ice V and the transition to ice XIII", *J. Chem. Phys.*, **129**(16):164513 (2008).

24. Chris Knight and Sherwin J. Singer, "A re-examination of the ice III/IX hydrogen bond ordering phase transition ", *J. Chem. Phys.*, **125**(6):064506 (2006).

25. Chris Knight, Sherwin J. Singer, Jer-Lai Kuo, Tomas K. Hirsch, Lars Ojamäe and Michael L. Klein, "Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions", *Phys. Rev. E*, **73**(5):056113 (2006).

26. Chris Knight and Sherwin J. Singer, "Prediction of a phase transition to a hydrogen bond ordered form of ice VI", *J. Phys. Chem. B*, **109**(44):21040 (2005).

27. Sherwin J. Singer, Jer-Lai Kuo, Tomas K. Hirsch, Chris Knight, Lars Ojamäe and Michael L. Klein, "Hydrogen bond topology and the ice VII/VIII and Ih/XI proton ordering phase transitions", *Phys. Rev. Lett.*, **94**(13):135701 (2005).

28. Christopher Knight and M. C. Milletti, "Theoretical characterization of two reaction pathways for the intramolecular cyclization of 2-(3-benzylaminopropanoyl-amino)benzamide", *J. Mol. Struct.: THEOCHEM*, **724**:143 (2005).

Conference Publications

1. Preeti Malakar, Venkatram Vishwanath, Christopher Knight, Todd Munson, Michael Papka, "Optimal Execution of Co-analysis for Large-scale Molecular Dynamics Simulations" In Proceedings of the International Conference for High Performance Computing, Network, Storage and Analysis (SC'16), November 2016, Salt Lake City, Utah, USA.

2. Preeti Malakar, Venkatram Vishwanath, Todd Munson, Christopher Knight, Mark Hereld, Sven Leyffer, Michael Papka, "Optimal scheduling of in-situ analysis for large-scale scientific simulations" In Proceedings of the International Conference for High Performance Computing, Network, Storage and Analysis (SC'15), November 2015, Austin, Texas, USA.

3. Nayong Kim, Richard Platania, Tom Keyes, Wei Huang, Chris Knight, Seun-jong Park, and Joohyun Kim, "Enabling Large-scale Biomolecular Conformation Search with Replica Exchange Statistical Temperature Molecular Dynamics (RESTMD) over HPC and Cloud Computing Resources" in *IEEE 29th International Conference on Advanced Information Networking and Applications Workshops (WAINA)*, 61-66 (2015).

4. Andrew M. Herring, Melissa A. Vandiver, Asley M. Maes, Himashu Sarode, E. Bryan Coughlin, Daniel M. Knauss, Yushan Yan, Gerrick E. Lindberg, Christopher Knight, Gregory A. Voth, Daniel Herbst, Thomas A. Witten, and Matthew W. Liberatore, "Fundamental Studies of Alkaline Exchange Membranes Towards Optimization in a Fuel Cell Environment", *ECS Trans.,* **50**(2): 2059-2066 (2012).

5. Gerrick E. Lindberg, Chris Knight, Lisa E. Feldberg, and Gregory A. Voth, "Molecular Dynamics Simulations of Hydroxide Solvation and Transport in Anionic Exchange Membranes", *ECS Trans.,* **50**(2): 2053-2058 (2012).

6. Yuxing Peng, Chris Knight, Philip Blood, Lonnie Crosby, Gregory A. Voth, "Extending Parallel Scalability of LAMMPS and Multiscale Reactive Molecular Simulations", XSEDE12, **37**:1-7 (ACM, New York, 2012).

7. Gerrick E. Lindberg, Chris Knight, Ryan Jorn, James F. Dama, and Gregory A. Voth, "Multiscale Simulation of Hydroxide Solvation and Transport in Anion Exchange Membranes", *ECS Trans.,* **41**(1):1785 (2011).

8. Himanshu Sarode, Melissa A. Vandiver, Ashley M. Maes, Benjamin Caire, James L. Horan, Yating Tan, Yifan Li, Gerrick E. Lindberg, James F. Dama, Chris Knight, Ryan Jorn, Martin E. Lenz, Robert Kasper, Shuang Gu, Bingzi Zhang, Sönke Seifert, Tsung-han Tsai, Wen X. Zhang, E. Bryan Coughlin, Daniel M. Knauss, Yushan Yan, Gregory A. Voth, Thomas A. Witten, Matthew W. Liberatore, and Andrew M. Herring, "Designing Alkaline Exchange Membranes from Scratch", *ECS Trans.,* **41**(1):1761 (2011).

9. Chris Knight and Sherwin J. Singer, "Theoretical study of a hydroxide ion within the ice-Ih lattice", *Physics and Chemistry of Ice* (Proceedings of the 11th International Conference on the Physics and Chemistry of Ice), ed., Werner F. Kuhs (Royal Soc. of Chemistry, 2007), p.339.

10. Chris Knight and Sherwin J. Singer, "Tackling the problem of hydrogen bond order and disorder", *Physics and Chemistry of Ice* (Proceedings of the 11th International Conference on the Physics and Chemistry of Ice), ed., Werner F. Kuhs (Royal Soc. of Chemistry, 2007), p.329.

Technical Reports

1. Adrian W. Lange, Gard Nelson, Christopher Knight, and Gregory A. Voth, "Multiscale Molecular Simulations at the Petascale (Parallelization of Reactive Force Field Model for Blue Gene/Q)", (*ALCF-2 Early Science Program Technical Report*), Argonne National Laboratory, 2013.

Presentations

1. "Science at ALCF: What has a supercomputer done for me lately?," Seminar presented at the Undergraduate Student Summer Research Lunch at Benedictine University, June 22, 2016.

2. "Algorithms for computationally efficient molecular simulations: chemical reactivity, predictive modeling of zeolites, and x-ray damage mechanisms," LANS Informal Seminar presented at Argonne National Laboratory, October 1, 2014.

3. "Algorithms for computationally efficient molecular simulations: chemical reactivity, predictive modeling of zeolites, and x-ray damage mechanisms," Seminar presented at the Argonne Leadership Computing Facility, Argonne National Laboratory, September 3, 2014.

4. "Computationally efficient reactive models derived from condensed phase ab initio simulations," Invited talk presented as the Technologies for Extreme Scale Computing seminar in the Center for Computation & Technology at Louisiana State University, July 17, 2014.

5. "Computationally efficient reactive models derived from condensed phase ab initio simulations", Seminar presented in the Chemistry Department at the University of Kansas, December 12, 2013.

6. "Rigorous route to interaction potentials for reactive models derived from condensed phase ab initio simulations", Talk presented at the 5th Annual Postdoctoral Research Symposium, Argonne National Laboratory, September 20, 2012.

7. "Rigorous route to interaction potentials for reactive models derived from condensed phase ab initio simulations", Invited talk presented at the 244th American Chemical Society National Meeting in symposium titled "Potential energy surface exploration in quantum chemistry" honoring Berny Schlegel, Philadelphia, PA, August 19-23, 2012.

8. "Extending Parallel Scalability of LAMMPS and Multiscale Reactive Simulations", Talk presented at XSEDE12, Chicago, IL, July 16-20, 2012.

9. "Defining reactive forcefields from condensed phase ab initio simulations", Poster presented at the Gordon Research Conference on Batteries, Ventura, CA, March 4-9, 2012.

10. "Defining reactive forcefields from condensed phase ab initio simulations", Poster presented at the American Conference on Theoretical Chemistry, Telluride, CO, July 17-22, 2011.

11. "Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice", Poster presented at 11th International Conference on the Physics and Chemistry of Ice, Bremerhaven, Germany, July 23-28, 2006.

12. "Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice", Talk presented at 38th Midwest Theoretical Chemistry Conference, Columbus, OH, June 15-17, 2006.

13. "Hydrogen bond topology, new interpretations of order/disorder transitions in ice, and the behavior of defects in a disordered ice lattice", Talk presented at Midwest Thermodynamics and Statistical Mechanics Conference, Akron, OH, May 25-26, 2006.

14. “Theoretical characterization of the potential energy surfaces of 2-(3-benzylamino-propanoylamino) benzamide”, Poster presented at 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003.

15. “Microwave synthesis and investigation of medium-sized ring systems containing nitrogen atoms”, Poster presented at 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003.

Workshops

1. Participation in the Nanoporous Materials Genome Center All-Hands meeting hosted by the University of Minnesota, October 2-3, 2015.

2. Participation in the 2015 Scientific Discovery through Advanced Computing (SciDAC-3) Principle Investigator Meeting, Bethesda, MD, July 22-24, 2015 and assisted with presenting dual-LCF (ALCF & OLCF) posters.

3. Participation in the Nanoporous Materials Genome Center All-Hands meeting hosted by the University of Minnesota, October 18-19, 2014.

4. Participation as an ALCF Catalyst at the ”Mira Performance Boot Camp” organized by the Argonne Leadership Computing Facility (ALCF), May 20-22, 2014, Argonne National Laboratory.

5. Invitation to participate in the ”7th Bishop’s Lodge Workshop: Materials for Energy Conversion” workshop organized by Plamen Atanassov (The University of New Mexico), November 3-5, 2013, Santa Fe, NM. Talk titled ”Progress towards a fundamental understanding of charge transport mechanisms in fuel cell membranes”.

6. Invitation to participate in the ”ONETEP Master Class 2013” workshop organized by the ONETEP Developers group, August 27-30, 2013, Cambridge, UK.

7. Participation in the ”Mira Performance Boot Camp” organized by the Argonne Leadership Computing Facility (ALCF), May 21-24, 2013, Argonne National Laboratory.

8. Talk titled ”Multiscale Molecular Simulations at the Petascale” at the ”Early Science Program Principle Investigators Meeting” organized by the Argonne Leadership Computing Facility (ALCF), May 15-16, 2013, Argonne National Laboratory.

9. Participation in the ”Mira Community Conference” organized by the Argonne Leadership Computing Facility (ALCF), March 4-8, 2013, Argonne National Laboratory.

10. Invitation to participate in the ”ONETEP Master Class 2012” workshop organized by the ONETEP Developers group, August 28-31, 2012, Cambridge, UK.

11. Invitation to participate in the ”Leadership Computing Platforms, Extreme-scale Applications, and Performance Strategies” workshop organized by the Center for Scalable Application Development Software (CScADS), July 23-26, 2012, Snowbird, UT.

12. Participation in the ”Early Science April Workshop - Code for Q” workshop organized by the Argonne Leadership Computing Facility (ALCF), April 30 - May 3, 2012, Argonne National Laboratory.

13. Participation in the ”ALCF 2012 Winter Workshop” organized by the Argonne Leadership Computing Facility (ALCF), January 23-26, 2012, Argonne National Laboratory.

14. Talk titled "Multiscale Molecular Simulations at the Petascale" at the "ALCF Early Science Program Kick-Off Workshop" organized by the Argonne Leadership Computing Facility (ALCF), October 18-19, 2010, Argonne National Laboratory.

DOE LCF Projects (excluding Director's Discretionary)

1. J. Ilja Siepmann, Laura Gagliardi, Christopher Knight, Christopher Mundy, Neeraj Rai, David Sholl, Randall Snurr, Donald Truhlar, and Yongchul Chung "Predictive Modeling of Functional Nanoporous Materials", 117 Million core-hours on Mira (ALCF), ALCC 2016-2017.

2. Marco Govoni, Alex Gaiduk, Hosung Seo, Christopher Knight, He Ma, Giulia Galli, and Francois Gygi, "Computational engineering of defects in soft and hard materials: energy and quantum information applications", 53.7 Million core-hours on Mira (ALCF), ALCC 2016-2017.

3. Phay Ho, Christopher Knight, Christoph Bostedt, and Linda Young, "Modeling of Intense X-ray Laser Dynamics in Nanoclusters", 10 Million core-hours on Mira (ALCF), ALCC 2016-2017.

4. Gregory A. Voth and Chris Knight, "Charge Transport in Thin FIlm Ionomers", 100 Million core-hours on Mira (ALCF), INCITE 2016.

5. Marco Govoni, Chris Knight, Giulia Galli, Francois Gygi, and Jonathan Skone, "First Principles Large Scale Simulations of Interfaces for Energy Conversion and Storage", 75 Million core-hours on Mira (ALCF), ALCC 2015-2016.

6. J. Ilja Siepmann, Michael W. Deem, Laura Gagliardi, Chris Knight, David S. Sholl, Randall Q. Snurr, and Donald G. Truhlar, "Predictive Modeling of Functional Nanoporous Materials", 120 Million core-hours on Mira (ALCF), ALCC 2015-2016.

7. Gregory A. Voth and Chris Knight, "Influence of Morphology on Proton Transport in Proton Exchange Membranes", 57.6 Million core-hours on Mira (ALCF), ALCC 2014-2015.